Analysis of Dislocation Nucleation from Crystal Surfaces

Guanshui Xu

Department of Mechanical Engineering
University of California at Riverside
Riverside, CA 92521
Email: gxu@engr.ucr.edu; Phone: (909) 787-2497; Fax: (909) 878-2899

Abstract

The energetics of dislocation nucleation from crystal surfaces is analyzed based on the Peierls-Nabarro dislocation model. The variational boundary integral approach is used to obtain the profiles of the embryonic dislocations in various three-dimensional nucleation configurations. The stress dependent activation energies required to activate dislocations from their stable to unstable saddle point configurations are determined. Compared to previous analyses of this type of problem based on continuum elastic dislocation theory, the presented analysis eliminates the uncertain core cutoff parameter by allowing for the existence of an extended dislocation core as the embryonic dislocation evolves. Moreover, atomic information can be incorporated to reveal the dependence of the nucleation process on the profile of the atomic interlayer potential as compared to continuum elastic dislocation theory in which only elastic constants and Burgers vector are relevant. The analysis of dislocation nucleation from surfaces of heterogeneities will be particularly discussed.